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13. ABSTRACT (Maximum 200 words)

We studied theoretically the electronic properties of single and vertically coupled InAs/GaAs self-assembled quantum dots (SAD) with a computational model which takes into account conduction-valence band mixing through an eight-band, strain dependent **k.p** hamiltonian. In single SADs, we showed that experimental photoluminescence peaks cannot be simply interpreted as transitions between harmonic oscillator states in the valence band and in the conduction band. We also provided a detailed account of electron-hole alignment as a function of external electric fields, SAD chemical composition, Ga diffusion profile in the dot and the dot shape. In particular, we invalidated the perturbation theory in the interpretation of the interband Stark effect. In vertically stacked coupled SADs, we specifically demonstrated the localization of hole states, even for vanishing dot separation. We also predicted the existence of an anomalous Stark effect for interband transitions. We also showed that intraband optical transitions between 1s and 2p bonding states in the conduction band, are strongly enhanced compared with similar transitions in single SADs. These transitions exhibit a strong asymmetric dependence in an external electric field, due to the SAD morphology. The intraband Stark effect also provides large tunability between electron states for mid-infrared transitions.

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Sincerely,

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Enclosure 3

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FINAL PROGRESS REPORT

1) Statement of the problem studied.

This research is dealing with a theoretical study of the electronic properties of single and vertically coupled self-assembled InGaAs/GaAs quantum dots (SADs). Our approach is based on an 8 band k.p Hamiltonian that takes into account the effect of strain between materials by a continuous model. We focus on the quantum mechanical coupling between vertically stacked SADs, and its response to an external electric field. The advantage of our numerical model is its flexibility in dealing with various SAD shapes, alloy InGaAs compositions and inhomogeneous stoichiometric profile.

2) Summary of the most important results

In testing our computational model on the experimental data of single SADs, important new results have been obtained which provide considerable insight in the electronic properties of these nanostructures . Asides from our physical findings, one of the original aspects of this work is the theoretical model itself that for the first time, integrates 3D k.p SAD modeling with strain, piezoelectricity and external electric field effects.

a) Interband optical transitions in single SADs.

Our k.p model was able to reproduce correctly the experimental optical spectra and optical anisotropy of SADs of similar sizes and shapes (e.g. by O.B. Shcheckin et al, APL 77, 466 (2000) and R. Heitz et al, PRB 62, 16881 (2000)). In addition, we demonstrated that the energy separation between hole states contributes to a significant fraction of the inter-band transition energies, thereby invalidating the effective mass two-dimensional harmonic oscillator model for the electronic structure of SADs. We also showed that aside from the ground state transition that is characterized by appreciable oscillator strength, other photoluminescence peaks in the experimental spectra are made of a significant number of equal-strength electron-hole transitions with no particular dominant transition.

b) Electron-hole alignment and QCSE in single SADs

We also investigated the influence of chemical composition and shape of InAs dots, on the electron-hole alignment as a function of the GaAs diffusion profile, and specifically showed that inverted alignment as suggested by P.W. Fry et al. (PRL 84, 2000, p.733), is indeed possible. However, this phenomenon is not universal, even for 100-oriented SADs, and is restricted to particular dot shapes and diffusion profiles. We also indicated significant deviations from the usual quadratic dependence of the ground state interband transition energy on applied electric fields in InAs/GaAs SADs. In particular, we showed that conventional second-order perturbation theory fails to correctly describe the Stark

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shift for electric field below F = 10 kV/cm in high dots, and were able to demonstrate this effect is predominantly due to the three-dimensional strain field distribution which for various dot shapes and stoichiometric compositions drastically affects the hole ground state. Our conclusions were supported by experiments.

c) Intra-band transitions and quantum confined Stark effect (QCSE) in coupled SADs

The main aspect of our research dealt with the electronic properties of vertically coupled SADs under the influence of an external electric field. We specifically showed that intra-band optical transitions, especially between the s-like and p-like orbitals, are significantly enhanced in double dots compared with similar transitions in single SADs. In addition to field-tunable transitions, we predicted a strong asymmetry in the oscillator strengths for positive and negative electric fields oriented along the growth direction. In collaboration with the group of Prof. M. Skolnick, University of Sheffield, U.K. we showed the " inversion" of selection rules for intra-band optical transitions in coupled SADs compared to single SADs. We are able to demonstrate that these effects result from the combined influence of strain and hole state mixing in the SAD conduction band spectrum.

d) Inter-band transitions and QCSE in coupled SADs

As a natural extension of this work, we also predicted an anomalous QCSE for inter-band transitions in vertically stacked SADs, which deviates strongly from the expected quadratic dependence on the electric field observed in quantum wells, for instance, which provides considerable insight into the effect of strain and hole mixing on the Stark-shifted optical transitions. We also predicted spontaneous localization of the hole states at all separation in vertically stacked SADs. This effect is due to the unique strain distribution that subjects the holes to a different environment than electrons in the conduction band. As a result, low energy hole are confined to their respective dot without forming bonding or anti-bonding states. We also showed that this localization plays the same role as a vertical electric field in coupled quantum systems, and substantially reduces the exciton binding energy, which may be an impediment to the formation of entangled states in quantum dot molecules.

3)Publications under ARO sponsorship:

a) Papers published in peer-reviewed journals:

1.Weidong Sheng and J. P. Leburton, *"Enhanced Intarband Stark Effect in Stacked InAsGaAs Self-Assembled Quantum Dots,"* Appl. Phys. Lett., 78, 1258 (2001).
2. Weidong Sheng and J. P. Leburton, *"Electron-Hole Alignment in InAs/GaAs Self-Assembled Quantum Dots: Effects of Chemical Composition and Dot Shape,"* Phys. Rev. B. RC. 63, 161301 (2001).
3. Weidong Sheng and J. P. Leburton, *"Enhanced Intraband Transitions with Strong Electric Field Asymmetry in Stacked InAs/GaAs Self-Assembled Quantum Dots,"* Phys. Rev. B. 64, 153302 (2001).

4. Weidong Sheng and J.P. Leburton, *"Anomalous Quantum Confined Stark Effect in Stacked InAs/GaAs Self-Assembled Quantum Dots,"* Phys Rev. Lett 88, 167401, 2002
5. Weidong Sheng and J.P. Leburton, *"Interband transition distribution in the optical spectra of InAs/GaAs self-assembled quantum dots"*, Appl. Phys. Lett. 80, 2755, (2002).
6. Weidong Sheng and J.P. Leburton,, *"Spontaneous localization in InAs/GaAs self-assembled quantum dot molecules"* Appl. Phys. Lett. 81, 4449 (2002); also in the December 9, 2002 issue of the Virtual Journal of Nanoscale Science & Technology.

b) Papers published in non-peer-reviewed journals or in conference proceedings

1.Weidong Sheng and J.P. Leburton, *"Enhanced Intraband Transitions in Stacked InAs/GaAs Self-Assembled Quantum Dots,"* Abstract booklet, 43rd Electronic Materials Conference, Notre Dame, IN, June 27-29, 2001, p.32.

2. Weidong Sheng and J.P. Leburton, *"Anomalous quantum confined Stark effects in vertically coupled InAs/GaAs self-assembled quantum dots,"* in Compound Semiconductors 2001, (Proceedings of the International Symposium on Compounds Semiconductors, Tokyo, Japan, October 1-4, 2001) IOP Conf. Series N0 170, Y Arakawa et al. Eds. pp 513-518.

3. Weidong Sheng and J. P. Leburton, *"2D-3D Transitions in the Quantum Stark Effect in Self-Assembled InAS/GaAs Quantum Dots"* Proc. of the ICSNN-02, Toulouse, France, July 21-26, 2002 in to be published in Physica E

4. Weidong Sheng and J.P. Leburton, *"Electronic properties of InAs/GaAs self-assembled quantum dots: Beyond the effective mass approximation"* in "Liber Amicorum" in honor of Prof. Devreese's 65th birthday, Phyisca Status Solidi (invited) (in press).

5.A.M.Adawi , E.A.Zibik , L.R.Wilson , A.Lemaitre, W.D.Sheng, J.W.Cockburn, M.S.Skolnick , J.P.Leburton, M.J.Steer, M.Hopkinson and G.Hill . *" Inversion of the intersublevel optical selection rule in strongly coupled InGaAs/GaAs self-assembled quantum dots"*, Proc. Of the 26th International Conference of the Physics of semiconductors (ICPS-26), July 29- Aug.2, 2002, Edinburgh, UK (in press)

c) Papers presented at meetings, but not published in conference proceedings

1.Weidong Cheng and J. P. Leburton, *"Effect of Gallium Diffusion in InAs/GaAs Self-Assembled Quantum Dots: Inverted Electron-Hole Alignment,"* Proc. Of the 28th Conference of the Physics and Chemistry of Semiconductor Interfaces (PCSI), Lake Bueno Vista, FL, Jan. 7-11, 2001.

2. Weidong Cheng and J.P. Leburton, " Quantum Stark Effect in self-Assembled InAs/GaAs Quantum dots" Advanced Heterostructure Workshop, Kona, Dec. 2-6, 2002, Kona, Hawaii,

d) Papers submitted, but not published

1.Weidong Sheng and J. P. Leburton, *"Absence of correlation between built-in electric dipole moment and quantum Stark effect in self-assembled inAs/GaAs quantum dots"* cond-mat 0204579; Phys Rev. B. (in review)

e) Technical reports submitted to ARO

1. Interim progress report for the period covering 4/1/99-12/31/99
2. Interim progress report for the period covering 1/1/00-12/31/00

3. Interim progress report for the period covering 1/1/01-12/31/01

4) Scientific personnel:
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5) Report of invention: None